Theoretica Chimica Acta

A Journal for Structure, Dynamics and Radiation

Volume 78 1990/91

EDITORS

Klaus Ruedenberg, Editor in Chief
Ames Laboratory USDOE and Department of Chemistry, Iowa State University, Ames, IA 50011, USA

David Chandler
Chemistry Department
University of California
Berkeley, CA 94720, USA

Ernest R. Davidson
Chemistry Department
University of Indiana
Bloomington, IN 47401, USA

Nicholas C. Handy
University Chemical Laboratory
Lensfield Road
Cambridge CB2 1EW, England

Joshua Jortner
Institute of Chemistry
Tel Aviv University
Ramat Aviv, Tel Aviv, Israel

Werner Kutzelnigg
Theoretical Chemistry Institute
Ruhr University
4630 Bochum 1, FRG

Josef Michl
Chemistry Department
University of Texas
Austin, TX 78712-1167, USA

William H. Miller
Chemistry Department
University of California
Berkeley, CA 94720, USA

Keiji Morokuma
Institute for Molecular Science
Myodaiji
Okazaki 444, Japan

Björn O. Roos
Department of Theoretical Chemistry
Chemical Centre, P. O. Box 124
University of Lund
S-22100 Lund, Sweden

Henry F. Schaefer III
Chemistry Department
University of Georgia
Athens, GA 30602, USA

Donald G. Truhlar
Chemistry Department
University of Minnesota
Minneapolis, MN 55455, USA

ADVISORY BOARD

R. Ahlrichs, Karlsruhe
V. Aquilanti, Perugia
R. J. Bartlett, Gainesville
M. V. Basilevsky, Moscow
M. S. Child, Oxford
K. F. Freed, Chicago
K. Fukui, Kyoto
E. J. Heller, Seattle
M. Karplus, Cambridge, Mass.
W. Kolos, Warsaw
W. Meyer, Kaiserslautern
M. D. Newton, Upton, New York
J. Paldus, Waterloo
L. Radom, Canberra
R. Zahradnik, Praha

SPRINGER INTERNATIONAL

Theoretica Chimica Acta

A Journal for
Structure, Dynamics and Radiation

Founded and edited in 1962 by H. Hartmann from Vol. 1 (1962) to Vol. 66 (1984).
As of Vol. 67 (1985) edited by K. Ruedenberg et al.

Copyright
Submission of a manuscript implies: that the work described has not been published before (except in the form of an abstract or as part of a published lecture, review, or thesis); that it is not under consideration for publication elsewhere; that its publication has been approved by all coauthors, if any, as well as by the responsible authorities at the institute where the work has been carried out; that, if and when the manuscript is accepted for publication, the authors agree to automatic transfer of the copyright to the (publisher, society); and that the manuscript will not be published elsewhere in any language without the consent of the copyright holders.
All articles published in this journal are protected by copyright, which covers the exclusive rights to reproduce and distribute the article (e.g., as offprints), as well as all translation rights. No material published in this journal may be reproduced photographically or stored on microfilm, in electronic data bases, video disks, etc., without first obtaining written permission from the publisher.
The use of general descriptive names, trade names, trademarks, etc., in this publication, even if not specifically identified, does not imply that these names are not protected by the relevant laws and regulations.
While the advice and information in this journal is believed to be true and accurate at the date of its going to press, neither the authors, the editors, nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Special regulations for photocopies in the USA

Photocopies may be made for personal or in-house use beyond the limitations stipulated under Section 107 or 108 of U.S. Copyright Law, provided a fee is paid. This fee is US $ 0.20 per page, or a minimum of US $ 1.00 if an article contains fewer than five pages. All fees should be paid to the Copyright Clearance Center, Inc., 21 Congress Street, Salem, MA 01970, USA, stating the ISSN 0040-5744, the volume, and the first and last page numbers of each article copied. The copyright owner's consent does not include copying for general distribution, promotion, new works, or resale. In these cases, specific written permission must first be obtained from the publisher.

Typesetter Datapage Int. Ltd., Dublin

Printers Brühlsche Universitätsdruckerei, Giessen, FRG

© Springer-Verlag Berlin Heidelberg 1991
Springer-Verlag GmbH & Co. KG, 1000 Berlin 33, FRG
Printed in Germany

Contents

Albuquerque LMPC → Costa Cabral BJ
Andrae D, Häußermann U, Dolg M, Stoll H, Preuß H: Energy-adfusted *ab initio* pseudopotentials for the second and third row transition elements: molecular test for M_2 (M = Ag, Au) and MH (M = Ru, Os) 247
Aoki S → Koga T
Asai Y → Tachibana A

Balasubramanian K: Generators of the character tables of generalized wreath product groups 31
Bone RGA, Handy NC: *Ab initio* studies of internal rotation barriers and vibrational frequencies of $(C_2H_2)_2$, $(CO_2)_2$, and C_2H_2—CO_2 133
Budeir RN → El-Issa BD

Costa Cabral BJ, Albuquerque LMPC, Silva Fernandes FMS: *Ab initio* study of the conformational equilibrium of ethylene glycol 271

Davidson ER → Tupper KJ
DeLin Shen, Pritchard HO: On the dynamics of free-radical disproportionation reactions 241
Dillon IP → Head JD
Dolg M → Andrae D

Elbert ST → Valtazanos P
Elbert ST → Xantheas S
El-Issa BD, Budeir RN: Stationary points on the aminomethanol potential energy surface 211

Fujita S: Application of coset representations to the construction of symmetry adapted functions 45

Gajewski JJ → Tupper KJ

Häußermann U → Andrae D
Handy NC → Bone RGA
Harcourt RD: Some valence bond calculations for H_2 with 1*s* and 2*s* basis sets 267
Head JD, Dillon IP: Utilization of 'pseudo-lattice symmetry' in cluster calculations 231
Hrušák J: An MNDO study of the electrophilic aromatic substitution on trifluor-obenzenes 203

Ikeuchi S → Tachibana A
Irie R: An approximate relation between Wigner—Seitz-type one-electron Hamiltonians and complete Hamiltonians for molecules and solids 11
Ishikawa S → Tachibana A

Knowles PJ → Werner H-J
Koga T, Aoki S: Charge and radial correlations in helium and helium-like atoms 165

Paldus J → Piecuch P
Pearson RG: Use of the chemical potential improve energies from approximate wave functions 281
Piecuch P, Paldus J: Coupled cluster approaches with an approximate account of triexcitations and the optimized inner projection technique. I. General orthogonally spin-adapted formalism 65
Preuß H → Andrae D
Pritchard HO → DeLin Shen
Ruedenberg K → Valtazanos P
Ruedenberg K → Xantheas S

Sadlej AJ → Urban M
Silva Fernandes FMS → Costa Cabral BJ
Stoll H → Andrae D

Tachibana A, Asai Y, Ikeuchi S, Ishikawa S, Yamabe T: Isomorphic electron orbitals for vibronic flexibility in a cyclopropenyl radical molecular device 1
Tupper KJ, Davidson ER, Gajewski JJ: The estimation of electron affinities form *ab initio* 1*s* orbital energies 25

Urban M, Sadlej AJ: Molecular properties in electronic excited states: multipole moments and polarizabilities of H_2O in the lowest $^1B_1$ and $^3B_1$ excited states 189

Valtazanos P, Elbert ST, Xantheas S, Ruedenberg K: The ring opening of cyclopropylidene to allene: global features of the reaction surface 287
Valtazanos P, Ruedenberg K: The ring opening of substituted cyclopropylidenes to substituted allenes: the effects of steric and long-range electrostatic interactions 397
Valtazanos P → Xantheas S

Wang Q-L → Zhan C-G
Werner H-J, Knowles PJ: A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations 175

Xantheas S, Valtazanos P, Ruedenberg K: The ring opening of cyclopropylidene to allene and the isomerization of allene: *ab initio* interpretation of the electronic rearrangements in terms of quasi atomic orbitals 327
Xantheas S, Elbert ST, Ruedenberg K: The ring opening of cyclopropylidene to allene: key features of the accurate reaction surface 365
Xantheas S → Valtazanos P

Yamabe T → Tachibana A

Zhan C-G, Wang Q-L, Zheng F: Calculation of the maximum bond order 129
Zheng F → Zhan C-G

Indexed in *Current Contents*